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CHALLENGES IN HAZARD IDENTIFICATION AUTOMATION

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Abstract

Process hazard analysis techniques are often very time-consuming tasks requiring experienced expert teams and thorough discussion meetings. Software tools for computer assistance in process hazard identification seem to be essential for the enhancement of these techniques and thus for the reduction of their time and labour requirements. Our work is focused on the development of such software tools implementing HAZOP (HAZard and OPerability) study and process simulations based on complex mathematical models. In this paper, challenges in hazard identification automation are discussed. Issues such as mathematical model parameter uncertainties and their impact on the safety analysis results, interpretation variability of quantitative HAZOP deviations for process simulations, limitations of built-in solvers in commercial process simulators for safety analysis and computing time dependence on the complexity of the mathematical model are discussed. As a part of this contribution, review of the application of a software tool developed by our research to novel industrial plants is demonstrated. Mathematical models of the considered case studies had various depths and included not only a reaction step, but also feed preparation and products separation steps. Output from the simulation-based HAZOP study carried out by the proposed tool is a simplified HAZOP-like report consisting of analysed HAZOP deviations and classification of their consequences.

Introduction

With the increasing level of automation in chemical industry, demand for implementation of complex hazard identification into a robust software solution had grew dramatically. Computer-aided hazard identification based on rigorous mathematical modelling of chemical processes represent a significant part in the research of hazard identification automation. In recent years, different approaches for incorporation of mathematical models were published, e.g. combination of safety engineering education and process simulation in MATLAB, analysis of process hazards in a novel three-phase hydrogenation reactor, risk assessment of membrane reactor for hydrogen production, advanced fault propagation study employing bifurcation analysis coupled with dynamic simulations, development of hazard identification extensions for industrially used commercial simulators etc.

Common denominator of these approaches is the adoption of HAZOP (HAZard and OPerability) study which is considered as one of the most used and complex hazard identification techniques in chemical industry. HAZOP study is a qualitative procedure to identify not only process hazards, but also operability problems based on generation of process parameter deviations from design intent by the logic combination of standardised guide words (NO, MORE, LESS, etc.) with suitable process parameters (pressure, flow, pump frequency, etc.)

In this paper, issues related to the use of software tool utilizing process simulations in commercial simulator and HAZOP study principles are discussed. Identification of these issues is based on the vast experience of the Department of Chemical and Biochemical Engineering of Slovak University of Technology with the development and application of such tool to case studies differing in depth and complexity. Commercial simulator is represented by a steady state simulator widely used for simulation of processes in gas and oil industry, Aspen HYSYS. Detailed analysis of obtained results of simulation-based HAZOP study performed by developed software tool is provided to determine the robustness of the proposed approach and to identify challenges associated with hazard identification automation.

Challenges in simulation-based HAZOP

Four main challenges related to implementation of the proposed simulation-based HAZOP approach into industrial practice were identified (Figure 1) based on previous experiences with its application. The goal of this contribution is to discuss following questions:

- How to properly define deviation?
- Is the mathematical model accurate enough?
- What are the limitations of numerical solving capabilities of commercial simulators?
- How long does it take to perform hazard identification based on process simulation?
Following four chapters are dedicated to detailed analysis of these questions and to formulation of suitable answers using knowledge gained by application of the developed software tool to three case studies and by verification of its results.

Figure 1. Challenges in hazard identification automation utilizing simulation-based HAZOP

Deviation definition

In conventional HAZOP study, HAZOP deviations are generated only by combining guide words and process parameters. The use of rigorous mathematical modelling and consequent computer simulations of the HAZOP deviations effect on the process operation, conventional HAZOP deviation is not sufficient as a simulation input. To start a simulation, a value of HAZOP deviation is required. Therefore, conventional procedure of HAZOP deviation generation has to be modified in order to obtain suitable simulation input. The amount of data necessary to be processed geometrically increases when the size is assigned to conventional HAZOP deviation. Furthermore, the increase is even more evident when the duration of HAZOP deviation is considered. Figure 2 illustrates the issue of proper HAZOP deviation for simulation-based HAZOP.

By assuming the HAZOP deviation size and duration, the possibility of overlooking process hazards can be reduced. Results from simulation-based HAZOP of case study of nitroglycerine production in continuous stirred tank reactor were analysed to demonstrate this effect. Detailed overview of mathematical model parameters and design intent conditions was introduced in our previous work in which the proposed software tool was able to identify hazardous consequence for a deviation of heat removal from reactor, i.e. cooling medium flow disturbance (Figure 3). Two qualitatively the same HAZOP deviations could lead to two qualitatively different consequences – Safe operating regime and hazardous operating regime caused by runaway effect. This phenomenon was observed only by considering also quantitative aspect of HAZOP deviation. Heat removal lower by 10 % led only to increased temperature in the reactor, with no possible runaway. However, for heat removal lower by 11 %, runaway could occur in the reactor. As it was depicted, it is important to define HAZOP deviations
properly in order to identify possible hazardous events that could be otherwise neglected by insufficient knowledge of the process by HAZOP team members.

![Diagram of Hazardous operating regime - runaway](image1)

Figure 3. Deviation definition effect on the quality of simulation-based HAZOP results in the case study of nitroglycerine production (square – design intent, x mark – limit runaway temperature, circle – last numerical solution in Aspen HYSYS)

**Model reliability**

The results of safety analysis based on process simulation can be significantly affected by the mathematical model parameter uncertainties\(^\text{16}\). Small change in sensitive model parameter value could lead to mislabelling safe operating regime as hazardous one and vice versa. This conclusion was supported by the analysis of model parameter uncertainties in case study of 3-methylpyridine N-oxidation\(^\text{17}\). N-oxidation operated in novel technology, closed continuous stirred tank reactor under elevated pressure, has to be carried out in small temperature interval to maintain process safety. Determination of the safety region boundaries was strongly dependent on the value of reaction enthalpy used in calculation. Figure 4 depicts the location of safe operating regime for combination of two process parameters, feed temperature and molar ratio of reactants in the feed stream, for five different values of reaction enthalpy. There was no such operating point that was satisfactory for every examined value of reaction enthalpy from the safety point of view. Additionally, only one of the identified economically optimised operating points for the original value of reaction enthalpy lied in the safe operating regime simulated for the reaction enthalpy value increased by 5%. If the original value of reaction enthalpy was underestimated, the process optimisation and safety analysis recommendations could cause dangerous operation of the process. Thus, mathematical model reliability and validity should always be thoroughly examined and the results of process simulation should always be verified.

**Solver capabilities**

Aspen HYSYS built-in solver employs advanced numerical solving procedures to ensure convergence of solution of differential-algebraic equations forming a mathematical model. However, its solving capabilities are limited in the case of strongly nonlinear process behaviour. To analyse this effect, case study of ammonia synthesis known for steady state multiplicity phenomenon was selected for hazard identification performed by the developed tool\(^\text{9}\). Detailed overview of mathematical model parameters and design intent was presented in previous papers\(^\text{9,14}\). Complete solution diagram for systems with steady state multiplicity could be compiled by using continuation and bifurcation analysis. It is necessary to employ such techniques to determine quality of steady states and to distinguish between stable and unstable steady states. However, using only Aspen HYSYS built-in solver, identification of at least part of the solution diagram is achievable. Figure 5a depicts the solution diagram obtained by process simulation in Aspen HYSYS. It was possible to simulate location of higher and lower solution branches that are composed of stable steady states. It was not possible to reveal process behaviour in the region created by unstable steady states. Because of the inability to affect the calculation process in Aspen HYSYS, own mathematical model of the ammonia synthesis reactor had to be created and continuation and bifurcation
analysis had to be applied to obtain complete solution diagram (Figure 5b). To complement hazard identification based on process simulation in Aspen HYSYS and to ensure completeness of the nonlinear process behaviour analysis, implementation of advanced numerical solving methods into the proposed software tool are crucial.

Figure 4. Effect of reaction enthalpy uncertainty on safe operating regime location (bright region – safe operating regime, dark region – hazardous operating regime)

Figure 5. Solution diagram of steady state multiplicity in ammonia synthesis obtained by simulation in Aspen HYSYS (a) and by continuation and bifurcation analysis (b)

Computing time

The last challenge in computer-aided hazard identification represent the compromise between mathematical model range and computing time requirements. The higher the number of unit operations in mathematical model, the longer the calculation lasts. Comparison between three different cases was made to analyse computing time dependence on the complexity of mathematical model. Case A was presented by simplified ammonia synthesis reactor model which was used also for previous analysis of Aspen HYSYS built-in solver capabilities. Case B presented ammonia synthesis model extended by steam reforming of natural gas and syngas purification unit\textsuperscript{18}. Model configuration for case C was identical to case B. The difference between case B and case C was the number of iterations allowed for calculation of recycled streams parameters. In the case B, the number of iterations was set to 10 iterations. In the case C, the number of iterations was increased a 100-fold,
to 1 000 iterations. Case A consisted of ca. 13 500 variables and 1 recycle stream with 10 iterations. Case B consisted of ca. 63 000 variables and 3 recycle streams with 10 iterations. Case C also consisted of ca. 63 000 variables and 3 recycle streams, but the number of iterations was set to 1 000. The convergence efficiency (Figure 6) and computing time (Figure 7) were monitored for computer simulations consisting of four HAZOP deviations in the interval of 1-30 % with the step of 1 % – “lower feed pressure”, “higher feed pressure”, “lower feed temperature” and “higher feed temperature”. The convergence efficiency was calculated as the number of correctly calculated steady states to overall number of simulations. The computing time represent time from the start of the simulation of the first HAZOP deviation to the end of the simulation procedure (simulation of the last HAZOP deviation and saving of steady state parameter values to the database). Figure 6 proves that increase in the number of iterations was necessary to ensure sufficient convergence efficiency. Figure 7 demonstrates how the computing time increased with increasing size of mathematical model (increasing number of variables to be calculated) and increasing number of iterations. Best results were achieved for the case A, however case A represented only simplified mathematical model of reviewed process and in case of requirement for more complex model to simulate whole plant, case A would not be satisfactory. In the case C, the 100-fold increase of iterations enabled convergence efficiency over 98 %, i.e. only 2 simulations were not calculated successfully.

![Figure 6](image1.png)

**Figure 6.** The convergence efficiency for cases A, B and C

![Figure 7](image2.png)

**Figure 7.** The computing time for cases A, B and C
Conclusion

In this contribution, four challenges in hazard identification automation based on rigorous mathematical modelling and process simulation were introduced and analysed. It was demonstrated how deviation definition, model reliability, solver capabilities and computing time can affect hazard analysis results. By assuming the HAZOP deviation size and duration, the scope of HAZOP study is significantly enhanced and the possibility of overlooking process hazards is reduced. However, if the HAZOP deviation size is not simulated in sufficient value range, hazardous consequences can remain unidentified. It was shown how mathematical model parameter uncertainties could lead to false conclusions from simulation-based HAZOP. Therefore, use of mathematical models in hazard identification requires always proper model verification. Solving capabilities of commercial simulators can also represent bottleneck in hazard identification automation. Limitations of built-in solvers in industrially used commercial simulators are more noticeable if the examined process exhibits strong nonlinear behaviour such as steady state multiplicity. In such case, implementation of advanced numerical algorithms seems to be crucial. In the last analysis, computing time dependence on the complexity and size of the mathematical model was studied. It was revealed that with increasing model complexity in the case of nonlinear processes, adjustments of calculation settings in the form of iterations number increase were necessary to ensure solution convergence. However, with a 100-fold increase of number of iterations, computing time have increased by almost 50%.

Computer-aided hazard identification based on rigorous mathematical modelling represent a suitable way for hazard identification automation. There are several phenomena challenging successful implementation of this approach into industrial practice and it is inevitable to properly address these challenges in order to achieve industrial application of software tools incorporating mathematical models and process simulation for safety assessment of chemical processes.

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Literature